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CANCERLIT is no longer being updated

METADEX enhancements

NEWS 43

Feb 13

NEWS 44 Feb 24

NEWS 45 Feb 24 PCTGEN now available on STN

NEWS 46 Feb 24 TEMA now available on STN

NEWS 47 Feb 26 NTIS now allows simultaneous left and right truncation

NEWS 48 Feb 26 PCTFULL now contains images

NEWS 49 Mar 04 SDI PACKAGE for monthly delivery of multifile SDI results

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CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),

AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002

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FILE CONTENT: 1907 - 16 Mar 2003 VOL 138 ISS 11

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This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=> s nitration reaction

5698 NITRATION 273267 REACTION

L2 28 NITRATION REACTION

(NITRATION (W) REACTION)

=> s 12 and microreactor

55 MICROREACTOR

L3 0 L2 AND MICROREACTOR

=> s 12 and micro?

5864 MICRO?

L4 1 L2 AND MICRO?

=> dis l4 bib abs

L4 ANSWER 1 OF 1 CASREACT COPYRIGHT 2003 ACS

AN 113:23454 CASREACT

- TI FK409, a novel vasodilator isolated from the acid-treated fermentation broth of Streptomyces griseosporeus. III. Reaction mechanism and synthesis
- AU Hino, Motohiro; Takase, Shigehiro; Itoh, Yoshikuni; Uchida, Itsuo; Okamoto, Masanori; Kohsaka, Masanobu; Aoki, Hatsuo; Imanaka, Hiroshi
- CS Explor. Res. Lab., Fujisawa Pharm. Co., Ltd., Tsukuba, 300-26, Japan
- SO Journal of Antibiotics (1989), 42(11), 1589-92 CODEN: JANTAJ; ISSN: 0021-8820
- DT Journal
- LA English
- AB FK409 [(E)-O2NCHMeCEt:CHC(:NOH)CONH2, I] was considered to be formed via a novel synchronous nitrosation-nitration reaction of FR-900411 [(2E,4E)-MeCH:CEtCH:CHCONH2, II] under acidic conditions with nitrite formed by microbial redn. of nitrate. Total synthesis of I was achieved starting from (E)-2-ethyl-2-butenal via a nitrosation reaction of II as a key step.

=> s 12 and pd<august 1999

361432 PD<AUGUST 1999

(PD<19990800)

L5 26 L2 AND PD<AUGUST 1999

=> s 15 not 14

L6 25 L5 NOT L4

=> dis 15 1-25 bib abs

- L5 ANSWER 1 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 132:151343 CASREACT
- TI A study of the reaction of different phenol substrates with nitric oxide and peroxynitrite
- AU Yenes, Susana; Messeguer, Angel
- CS Department of Biological Organic Chemistry, IIQAB (CSIC), Barcelona, 08034, Spain
- SO Tetrahedron (1999), 55(49), 14111-14122 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier Science Ltd.
- DT Journal
- LA English

GI

AB The reactivity of different phenol substrates, e.g., 4-ClC6H4OH, with nitric oxide and peroxynitrite was investigated. In general, nitration is the major reaction with peroxynitrite, while reactions with aq. solns. of nitric oxide led to mixts. of nitro and nitroso derivs. depending upon the phenol. Nitrosation occurs on phenol substrates bearing a free para-position with respect to the OH group with the exception of 1-naphthol, which afforded a 1:1 mixt. of the 2- and the 4-nitroso derivs. Chromans I and II showed the highest reactivity with peroxynitrite, which suggests that they can act as efficient scavengers of this toxic intermediate. In both cases the corresponding 5-nitro deriv. was the only reaction product detected. Finally, the fact that chroman II reacts with nitric oxide to afford the p-quinone deriv. III in 90% yield suggests that this antioxidant could also be of potential use as specific nitric oxide tracer in biol. tissues.

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 2 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 130:209610 CASREACT
- TI Furopyridines. XXVIII. Reactions of 3-bromo derivatives of furo[2,3-b]-, -[3,2-b]-, -[2,3-c]- and -[3,2-c]pyridine and their N-oxides
- AU Yamaguchi, Seiji; Awajima, Kazuaki; Hirai, Yoshiro; Yokoyama, Hajime; Shiotani, Shunsaku
- CS Department of Chemistry, Faculty of Science, Toyama University, Toyama, 930, Japan
- SO Journal of Heterocyclic Chemistry (1998), 35(6), 1249-1255 CODEN: JHTCAD; ISSN: 0022-152X
- PB HeteroCorporation
- DT Journal
- LA English
- AB Bromination of 3-bromofuro[2,3-b]pyridine, 3-bromofuro[3,2-b]pyridine and 3-bromofuro[3,2-c]pyridine afforded the 2,3-dibromo derivs., while 3-bromofuro[2,3-c]-pyridine did not give the dibromo deriv. Nitration of these compds. gave 2-nitro-3-bromo compds. The N-oxides of the title compds. were submitted to the cyanation with trimethylsilyl cyanide to yield corresponding .alpha.-cyanopyridine compds. Chlorination of bromofuropyridines with phosphorus oxychloride gave chloropyridine derivs. or chlorofuran derivs. Acetoxylation of bromofuropyridine oxides with acetic anhydride yielded acetoxypyridine compds.
- RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 3 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 130:196745 CASREACT
- TI 2-Nitroferrocenyloxazolines: precursors to nitrofulvalenes and derivatives of (pS) and (pR) -2-aminoferrocenecarboxylic acids
- AU Salter, Rhys; Pickett, Tom E.; Richards, Christopher J.
- CS Department of Chemistry, Cardiff University, Cardiff, CF1 3TB, UK
- SO Tetrahedron: Asymmetry (1998), 9(23), 4239-4247 CODEN: TASYE3; ISSN: 0957-4166
- PB Elsevier Science Ltd.
- DT Journal
- LA English
- AB Diastereoselective lithiation of (S)-2-ferrocenyl-4-(1-methylethyl)oxazoline, followed by addn. of N2O4, gave (S)-2-[(pS)-2-nitroferrocenyl]-4-(1-methylethyl)oxazoline which was subsequently converted into derivs. of (pS)-2-aminoferrocenecarboxylic acid. The corresponding (pR)-derivs. were obtained through use of a removable TMS blocking group. The 2-nitroferrocenyloxazolines produced in this work underwent facile photo-decomplexation to give 2-nitrocyclopentadienyliden-1,3-oxazolidenes.
- RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L5 ANSWER 4 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 128:167195 CASREACT
- TI Reactions of bridged halosubstituted adamantane derivatives with nitric acid
- AU Klimochkin, Yu. N.; Leonova, M. V.; Moiseev, I. K.; Aleksandrov, A. M.
- CS Samara State Technical University, Samara, 443056, Russia
- SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1997), 33(3), 340-344
 CODEN: RJOCEQ; ISSN: 1070-4280
- PB MAIK Nauka/Interperiodica Publishing
- DT Journal
- LA English
- AB Reactions of bridged halosubstituted adamantane derivs. with nitric acid result in nitrolysis products. In the presence of acetic anhydride, the reactions proceed at nodal positions to form nitroxy derivs., while in the case of 2,2-dichloroadamantane, the formation of a 1,4,4-trichlorosubstituted deriv. is obsd. The nitroxylation of 2-fluoroadamantane results in the formation of predominantly products with the cis-configuration.
- RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L5 ANSWER 5 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 128:167194 CASREACT
- TI Nitroxylation of 2-substituted adamantane derivatives
- AU Klimochkin, Yu. N.; Leonova, M. V.; Moiseev, I. K.
- CS Samara State Technical University, Samara, 443056, Russia
- SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1997), 33(3), 334-339 CODEN: RJOCEQ; ISSN: 1070-4280
- PB MAIK Nauka/Interperiodica Publishing
- DT Journal
- LA English

AB The reactions of bridged alkyladamantanes with nitric acid result in a mixt. of 1,2-nitroxy and 1,4-nitroxy, hydroxy, and nitro derivs., while nitroxylation of compds. with electron-withdrawing substituents in the bridging position gives only the corresponding 5-nitroxy derivs. Substituted adamantanes were characterized by the predominant formation of products with a Z-configuration. The comparative reactivity of 2-substituted adamantane derivs. in the reactions with nitric acid was detd. Correlations between logkapp of the nitroxylation of 2-R-adamantanes and the induction Taft .sigma.*-consts. were established.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L5 ANSWER 6 OF 26 CASREACT COPYRIGHT 2003 ACS
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AN 125:114649 CASREACT

TI syntheses and activities of 6-heterocyclyl-1-(substituted phenyl)benzotriazole herbicidal agents

IN Condon, Michael E.; Crews, Alvin D., Jr.; Manfredi, Mark C.

PA American Cyanamid Co., USA

SO U.S., 38 pp. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

1 1111	C14 1 2					
	PATENT NO.	KIND	DATE	APPLICATI	ON NO.	DATE
ΡI	US 5523277	Α	19960604	US 1995-3	87140	19950210
	US 5496954	Α	19960305	US 1995-4	37099	19950505
	US 5545742	Α	19960813	US 1995-4	37112	19950505
	ZA 9600901	Α	19970805	ZA 1996-9	01	19960205
PRAI	US 1995-387140	19950210				
os	MARPAT 125:11464	9				
GI						

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB A multistep process for the synthesis of a 6-heterocyclyl-1-(substituted phenyl) benzotriazole having the structural formula I comprises the condensation of [(benzotriazolyl)phenoxy]propionate, e.g., II [e.g., R1 = OCHMeCO2Me (1), OMe, OCF3, NMe2, Me] [in which II were prepd. from cyclocondensation of Me 2-[p-(acetamido-2-amino-4-fluoroanilino)phenoxy]propionate and Na nitrite] with 3,4,5,6-tetrahydrophthalic anhydride (2). E.g., a soln. of 1 and 2 in HOAc is refluxed for 24 h to give 6-heterocyclyl-1-(substituted phenyl)benzotriazole III. (Phenyl)benzotriazoles I (e.g., III) were tested for herbicidal activity which comprised applying the compd. to the foliage of the plants or to the soil or H2O contg. seeds or other propagating organs thereof at a rate of .apprx.0.016 kg/ha to 4.0 kg/ha.

L5 ANSWER 7 OF 26 CASREACT COPYRIGHT 2003 ACS

AN 124:342842 CASREACT

TI Nitration of benzene to dinitrobenzene and mononitrobenzene using anhydrous nitric acid in the absence of sulfuric acid or aprotic dipolar solvent

IN Mason, Robert W.

PA Olin Corp., USA

SO U.S., 4 pp., Cont.-in-part of U.S. 5,354,924.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 4

PATENT NO. KIND DATE APPLICATION NO. DATE ____ US 5488187 Α PΙ 19960130 US 1994-290575 19940815 US 5354924 19941011 US 1993-108035 19930817 Α PRAI US 1988-210549 19880622 US 1993-108035 19930817 US 1992-900213 19920617

AB A process is claimed for nitrating benzene to produce dinitrobenzene by a liq. phase nitration reaction of anhyd. nitric acid (designate nitric acid having an acid concn. of between 95 and 100 wt. %, preferably at least 98 wt. %, the remainder being water) with benzene in a reactor at a reaction temp. of between 30.degree. and 70.degree., and a reaction pressure not exceeding atm. pressure, said reaction employing a molar ratio of nitric acid plus any water to benzene of between 15:1 and 25:1, said reaction being conducted in the absence of sulfuric acid, and in the absence of any aprotic dipolar solvent during the reaction and in the absence of any aprotic dipolar solvent to halt the reaction, to produce said dinitrobenzene in a product mixt., followed by vacuum distn. of the product mixt., in the absence of any aprotic dipolar solvent, to remove unreacted nitric acid from said product mixt. thereby providing a dinitrobenzene product. In another aspect, the present invention relates to a process for nitrating benzene to produce mononitrobenzene by a liq. phase nitration reaction of anhyd. nitric acid with benzene in a reactor at a reaction temp. of between 0.degree. and 60.degree., and a reaction pressure not exceeding atm. pressure, for a reaction time that is preferably less than 15 (more preferably less than 5) minutes, said reaction employing a molar ratio of nitric acid plus any water to benzene of between 2:1 and 4:1, said reaction being conducted in the absence of sulfuric acid, and in the absence of any aprotic dipolar solvent as described above. The following illustrates dinitration: a magnetically stirred soln. of 55.07 g (0.857 mol) of 98% nitric acid in a 100 mL flask was chilled in a water bath; benzene (3.71 g, 0.048 mol) was injected subsurface to the nitric acid at 0.75 mL/min (mol ratio of nitric acid plus water to benzene = 18:1); extn. with CH2Cl2 followed by GC anal. indicated complete conversion in < 1 h (mononitrobenzene content < 200 ppm, trinitrophenol content of 200 ppm) and dinitrobenzene isomer ratio 1,2:1,3:1,4 = 9.6:88.3:2.0. The following illustrates mononitration: to a 4 mL glass vial was fed 7.0 mL of 98 % HNO3 (10.5 g, 0.163 mol of HNO3) and 5.0 mL benzene (4.39 g, 0.056 mol of benzene) at feed rates of 0.22 mL/min and 0.135 mL/min, resp.; the reactor content was adjusted to 2 mL (mean reaction residence time of 2.8 min); the reactor water bath was maintained at 15.degree. (.+-. 5.degree.); extn. with CH2Cl2 was followed by GC anal. which indicated recovery of 0.047 mol (83 %) of nitrobenzene.

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L5 ANSWER 8 OF 26 CASREACT COPYRIGHT 2003 ACS
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AN 123:169503 CASREACT

TI Method for producing aminocarbazole derivatives

IN Kamikawa, Taku; Maruyama, Osamu

PA Sumitomo Chemical Co, Japan

SO Jpn. Kokai Tokkyo Koho, 3 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO. KIND DATE APPLICATION NO. DATE

PI JP 07133261 A2 19950523 JP 1993-282636 19931111

PRAI JP 1993-282636 19931111

Aminocarbazole derives., useful as intermediates for dyes or pigments, are prepd. by catalytic hydrogenation of nitrocarbazoles in the presence of Fe-contg. Ni (1-40 wt.% Fe-Ni) catalyst and an alkali in an inert solvent. The preferred nitrocarbazole derivs. are 1- or 3-nitro-9-(lower alkyl)carbazoles. This process can directly use nitrocarbazole derivs. isolated by regular procedures from a nitration reaction mixt. and the redn. is not interfered and slowed down by impurities such as NO3 ions in the raw material nitrocarbazole derivs. and thereby does not result in low yields. Thus, 100 g 9-ethylcarbazole was nitrated by concd. HNO3 in 245 g o-dichlorobenzene and the reaction mixt. was neutralized with 10% aq. NaOH, followed by sepg. the oil layer and washing it with warm water to give a soln. (370 g) contg. 110.0 g 3-nitro-9-ethylcarbazole (90% yield), 8.0 g 1-nitro-9-ethylcarbazole, and NO3- 30 ppm in o-dichlorobenzene. The latter soln. 375, H2O 115, NaOH 1.0, and Raney Ni (30 wt.% Fe) 2.2 g were added to an autoclave, hydrogenated under H pressure 8 kg/cm2.G at 80.degree. with stirring for 3 h, cooled to 70.degree., and filtered to give, after sepn. of the aq. layer, a soln. (345 g) of 3-amino-9-ethylcarbazole in o-dichlorobenzene in 98% yield. Hydrogenation of the same soln. in the presence of Raney Ni without Fe and FeSO4 at 80.degree. and H pressure 8 kg/cm2.G for 14 h gave 3-amino-9-ethylcarbazole in 87% yield.

- L5 ANSWER 9 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 123:55613 CASREACT
- TI Nitration by oxides of nitrogen. 9. Preparation of nitramine-nitrates by ring-opening nitration of azetidines by dinitrogen pentoxide (N2O5)
- AU Golding, Peter; Millar, Ross W.; Paul, Norman C.; Richards, David H.
- CS Defense Res. Agency, Kent, TN14 7BP, UK
- SO Tetrahedron (1995), 51(17), 5073-82 CODEN: TETRAB; ISSN: 0040-4020
- PB Elsevier
- DT Journal
- LA English
- Eleven azetidines, bearing various types of substituents on the ring nitrogen, were treated with N2O5 in chlorinated solvents at sub-ambient temp. and in certain cases formed 1,3-nitramine-nitrate products by a novel ring-opening nitration reaction analogous to that established for aziridines. Yields of the nitramine-nitrates, where ring-opening took place, were generally moderate to high (41-88 %), but azetidines bearing N-acyl substituents (acetyl, butyryl or carbamyl) instead underwent nitrolysis of the exocyclic substituent to form N-nitroazetidine. Also, azetidines bearing strongly electron-withdrawing groups such as picryl were inert to attack by N2O5. The different reactivity of azetidines compared with aziridines is rationalized in terms of the reduced ring strain of the four-membered ring compds.
- L5 ANSWER 10 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 122:265918 CASREACT
- TI A New Route to 15N-Labeled, N-Alkyl, and N-Amino Nucleosides via N-Nitration of Uridines and Inosines
- AU Ariza, Xavier; Bou, Valenti; Vilarrasa, Jaume
- CS Faculty of Chemistry, University of Barcelona, Barcelona, 08028, Spain
- SO Journal of the American Chemical Society (1995), 117(13), 3665-73

CODEN: JACSAT; ISSN: 0002-7863

- PB American Chemical Society
- DT Journal
- LA English
- An novel method for the specific [3-15N]-labeling of pyrimidine nucleosides and [1-15N]-labeling of purine nucleosides is reported. The Nnitration reaction is carried out in good yields with
 nitronium trifluoroacetate in cold dichloromethane. Treatment of the
 resulting N-nitro nucleosides with 15NH3, alkylamines, or hydrazine
 cleaves the pyrimidine ring at room temp., affording open intermediates
 which undergo cyclization to 15N-labeled, N-alkylated, or N-amino
 nucleosides, resp. Prepn. of [1-15N]adenosine from inosine in a 52%
 overall yield is illustrative of the scope of the procedure.
 [3-15N,15NH2]-5'-O-Acetyl-3-amino-2',3'-O-isopropylideneuridine and
 [1-15N,15NH2]-2',3',5'-tri-O-acetyl-1-aminoinosine have also been obtained
 from double labeled hydrazine. By using a 15N-labeled substrate and/or
 15N-labeled benzylamine it is shown that the amine attack takes mainly
 place at C4 of uridine and at C2 of inosine.
- L5 ANSWER 11 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 120:53917 CASREACT
- TI Nitration by oxides of nitrogen. Part 6. Preparation of di- and polynitrates by ring-opening nitration of epoxides by dinitrogen pentoxide (N2O5)
- AU Golding, Peter; Millar, Ross W.; Paul, Norman C.; Richards, David H.
- CS Def. Res. Agency, Fort Halstead/Sevenoaks/Kent, TN14 7BP, UK
- SO Tetrahedron (1993), 49(32), 7037-50 CODEN: TETRAB; ISSN: 0040-4020
- DT Journal
- LA English
- AB Eighteen epoxides were treated with N2O5 in chlorinated hydrocarbon solvents (principally CH2Cl2) to give vicinal nitrate ester products by a novel ring-opening nitration reaction. The procedure offers easier temp. control and simpler isolation procedures compared with conventional mixed-acid nitrations; it also enables selective nitrations to be carried out on polyfunctional substrates. The scope and limitations of the reaction, as well as those of an alternative route utilizing N2O4 with in situ oxidn. of an intermediate nitrite-nitrate, are discussed.
- L5 ANSWER 12 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 114:228678 CASREACT
- TI Aprotic nitration (NO2+BF4-, nitryl tetrafluoroborate) of 2-halo- and 2,6-dihalopyridines and transfer-nitration chemistry of their N-nitropyridinium cations

- AU Duffy, Joseph L.; Laali, Kenneth K.
- CS Dep. Chem., Kent State Univ., Kent, OH, 44242, USA
- SO Journal of Organic Chemistry (1991), 56(9), 3006-9 CODEN: JOCEAH; ISSN: 0022-3263
- DT Journal
- LA English
- GΙ

AΒ NO2+BF4- nitration of 2,6-dibromo- and 2,6-dichloropyridine in CH3CN results in predominant C-nitration, whereas in CH2Cl2, N-nitration is predominant. With 2,6-difluoropyridine only C-nitration is obsd. Dehalogenation of the C-nitrated derivs. affords 3-nitropyridine in moderate but greatly improved yields over conventional protic nitration of pyridine. Despite favorable steric inhibition to resonance and the -I effects of halogens, N-nitrated pyridinium salts I (X = Br, Cl) do not transfer-nitrate to aroms, even under forcing conditions. The lack of transfer-nitration reactivity is not due to in situ rearrangement of the nitro onium ions to nitrito onium ions. A mechanism involving neighboring group participation by the 2,6-halogens is proposed. The monohalo-N-nitropyridinium cations transfer-nitrate toluene and benzene. Transfer-nitration selectivities of the 2-bromo- and 2-chloro-Nnitropyridinium cations are comparable (KT/KB = 41-44), but the 2-fluoro-N-nitro cation is much less selective (more reactive) (KT/KB = 15.4), indicative of a stronger -I effect, weakening the N-N bond.

L5 ANSWER 13 OF 26 CASREACT COPYRIGHT 2003 ACS

AN 113:23454 CASREACT

TI FK409, a novel vasodilator isolated from the acid-treated fermentation broth of Streptomyces griseosporeus. III. Reaction mechanism and synthesis

AU Hino, Motohiro; Takase, Shigehiro; Itoh, Yoshikuni; Uchida, Itsuo; Okamoto, Masanori; Kohsaka, Masanobu; Aoki, Hatsuo; Imanaka, Hiroshi

CS Explor. Res. Lab., Fujisawa Pharm. Co., Ltd., Tsukuba, 300-26, Japan

SO Journal of Antibiotics (1989), 42(11), 1589-92 CODEN: JANTAJ; ISSN: 0021-8820

DT Journal

LA English

AB FK409 [(E)-O2NCHMeCEt:CHC(:NOH)CONH2, I] was considered to be formed via a novel synchronous nitrosation-nitration reaction of FR-900411 [(2E,4E)-MeCH:CEtCH:CHCONH2, II] under acidic conditions with nitrite formed by microbial redn. of nitrate. Total synthesis of I was achieved starting from (E)-2-ethyl-2-butenal via a nitrosation reaction of II as a key step.

L5 ANSWER 14 OF 26 CASREACT COPYRIGHT 2003 ACS

AN 112:219231 CASREACT

TI Manufacture of 1-nitroanthraquinone

IN Muszynski, Miroslaw

PA Osrodek Badawczo-Rozwojowy Przemyslu Barwnikow "Organika", Pol.

SO Pol., 4 pp. CODEN: POXXA7

DT Patent

LA Polish

FAN.CNT 1

 PRAI PL 1983-243478 19830818

- The title compd. (I) is produced by nitration of a 5-50% anthraquinone (II) soln. or suspension in .gtoreq.70% H2SO4 or oleum contg. .ltoreq.65% SO3 by using a 5-50% aq. inorg. nitrate soln. at a nitrate/II mol ratio (1.0-2.5):1 and at -10 to +120.degree.. Preferably, the nitrate is NaNO3, KNO3, Ca(NO3)2, and/or Al(NO3)3. Purity of the resulting I is >90% which is satisfactory for manuf. of 1-aminoanthraquinone and further dye intermediates. Thus, the nitration reaction was done in a cascade of 4 reactors where a 10% II soln. in 100% H2SO4 at 20.8 parts/min and 30% aq. KNO3 soln. at 4.5 parts/min were fed into the 1st 1 m3 reactor, and in the 2nd reactor, 65% oleum was added at 5 parts/min, and in the 4th reactor, water was added at 50 parts/min, with temps. in the 1st, 2nd, 3rd, and 4th reactors 35-45.degree., 65-75.degree., 90.degree., and 30.degree., resp. The product was withdrawn, filtered on a rotary filter, washed with water to pH 7, and dried to give I (purity 93%) at 25 parts/min.
- L5 ANSWER 15 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 112:51866 CASREACT
- TI Structure and synthesis of FK409, a novel vasodilator isolated from Streptomyces as a semi-artificial fermentation product
- AU Hino, Motohiro; Takase, Shigehiro; Itoh, Yoshikuni; Uchida, Itsuo; Okamoto, Masanori; Hashimoto, Masashi; Kohsaka, Masanobu
- CS Explor. Res. Lab., Fujisawa Pharm. Co., Tsukuba, 300-26, Japan
- SO Chemical & Pharmaceutical Bulletin (1989), 37(10), 2864-6 CODEN: CPBTAL; ISSN: 0009-2363
- DT Journal
- LA English
- AB The structures of FK409, a semi-artificial fermn. product and its precursor 4-ethylhexa-2,4-dienamide (I), were established by chem. and spectroscopic evidence and confirmed by conversion of I to FK409 via a synchronous nitrosation-nitration reaction.
- L5 ANSWER 16 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 111:186494 CASREACT
- TI Assessment of on-line nitration reactions as a means of determining nitrate by reversed-flow injection with reductive amperometric detection at a glassy carbon electrode
- AU Fogg, Arnold G.; Scullion, S. Paul; Edmonds, Tony E.
- CS Chem. Dep., Loughborough Univ. Technol., Loughborough/Leicestershire, LE11 3TU. UK
- SO Analyst (Cambridge, United Kingdom) (1989), 114(5), 579-81 CODEN: ANALAO; ISSN: 0003-2654
- DT Journal
- LA English
- AB Five compds. were investigated for use as online reagents in concd. H2SO4 for the reductive reversed flow-injection amperometric detn. of nitrate as a nitro deriv. at a glassy carbon electrode. The H2SO4 was dild. rapidly on injecting reagent soln. into a sample carrier stream and therefore the nitration reaction, which generally only takes place at H2SO4 concns. of greater than about 70%, had to be rapid. Thiophene-2-carboxylic acid was found to be the most suitable reagent of those studied. The nitration reaction was sufficiently rapid and the first of two redn. steps was at -0.19 V vs. SCE as indicated by linear sweep voltammetry; hence the detn. was free from interference by dissolved oxygen. Problems assocd. with contamination of the electrode surface with redn. product, which caused loss of signal after making repeated injections over an extended period, remained.

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ANSWER 17 OF 26 CASREACT COPYRIGHT 2003 ACS
L5
AN
    109:233186 CASREACT
    Separation of sulfuric and nitric acids from dinitrotoluene-containing
TI
     toluene nitration reaction mixtures by water addition
    Witt, Harro; Beckhaus, Heiko
ΙN
    Bayer A.-G., Fed. Rep. Ger.
Ger. Offen., 3 pp.
PΑ
SO
     CODEN: GWXXBX
DT
    Patent
LΑ
    German
FAN.CNT 1
                                          APPLICATION NO. DATE
                    KIND DATE
    PATENT NO.
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                                           DE 1987-3705091 19870218
PΙ
    DE 3705091
                      A1
                            19880901
                                           EP 1988-101799 19880208
    EP 279312
                      A2
                            19880824
    EP 279312
                       A3
                            19900425
    EP 279312
                      В1
                            19920506
        R: BE, DE, ES, FR, IT
     ES 2031167
                 T3 19921201
                                           ES 1988-101799
                                                             19880208
                                           US 1988-155199
                                                             19880212
    US 5001286
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                            19910319
                                           JP 1988-32001
                                                            19880216
     JP 63203650
                       A2
                            19880823
     JP 2640956
                      B2
                            19970813
PRAI DE 1987-3705091 19870218
     In the manuf. of dinitrotoluene, toluene nitration
     reaction mixts., after removal of the major portion of H2SO4 and
     HNO3, still contain .ltoreq.5% HNO3 and .ltoreq.6% H2SO4. By addn. of
     .ltoreq.10% H2O (based on dinitrotoluene content) to the nitration
     reaction mixt., a phase sepn. is produced and the remainder of the
     acids are removed in the aq. phase.
     ANSWER 18 OF 26 CASREACT COPYRIGHT 2003 ACS
L5
     107:22931 CASREACT
AN
     Some features characterizing the nitration reaction of
ΤI
     secondary polynitroalkanes
     Eremenko, L. T.; Oreshko, G. V.; Fadeev, M. A. Otd. Inst. Khim. Fiz., Chernogolovka, USSR
ΑU
CS
     Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya (1986), (6),
SO
     1357-61
     CODEN: IASKA6; ISSN: 0002-3353
DT
     Journal
LA
     Russian
     Nitration of pyridinium salts of (O2N) 2CRCH2CH(NO2) CH2CR(NO2) 2 (R = NO2,
AB
     F) with HNO3, HNO3-H2SO4, aq. HNO3, N2O4, NO2BF4, and ClNO2 was studied.
     Products and product ratios varied widely with reagents and reagent
     concns.
     ANSWER 19 OF 26 CASREACT COPYRIGHT 2003 ACS
L5
     96:6667 CASREACT
AN
     Oxidation state of cation radicals in the nitration
TI
     reaction of phenothiazine by nitric acid
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Morkovnik, A. S.; Dobaeva, N. M.; Okhlobystin, O. Yu.

Khimiya Geterotsiklicheskikh Soedinenii (1981), (9), 1214-16

Rostov Gos. Univ., Rostov, 344006, USSR

CODEN: KGSSAQ; ISSN: 0453-8234

Page 12

Journal Russian

ΑU

CS SO

DT

LΑ

- AB Nitration of phenothiazine by HNO3-HClO4 gave 78% cation radical I which was oxidized by HNO3 to give 68% phenothiazonium perchlorate II. Further nitration gave 81% III (n = 1) via III (n = 0).
- L5 ANSWER 20 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 84:30013 CASREACT
- TI Halosubstituted phenylcyclopropanes in a nitration reaction
- AU Shabarov, Yu. S.; Mochalov, S. S.; Novokreshchennykh, V. D.; Volkov, E. M.; Ermishkina, S. A.
- CS Mosk. Gos. Univ. im. Lomonosova, Moscow, USSR
- SO Zhurnal Organicheskoi Khimii (1975), 11(9), 1907-13 CODEN: ZORKAE; ISSN: 0514-7492
- DT Journal
- LA Russian
- GI For diagram(s), see printed CA Issue.
- AB Nitration of I in Ac20 gave 40% II, 23% III and 9% IV. Nitration of V (X = Cl, Br) gave 33-51.9% VI and 31.7-43.8% VII; nitration of V (X = iodo) gave 11.4% VI, 16.8% VII, 53% (2-nitrophenyl)cyclopropane, 5.5% 1-(2-iodophenyl)-1,3-propanediol dinitrate, and 5.4% 1-acetoxy-1-(2-iodophenyl)-3-propanol. The orientation of the NO2 was detd. by the cyclopropyl ring. Several of the cyclopropylhalonitrobenzenes were isomerized.
- L5 ANSWER 21 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 84:4749 CASREACT
- TI Nitration of furan derivatives by acetylnitrate. I. Products of the nitration of the methyl ester of furan-2-carboxylic acid
- AU Lola, D.; Venters, K.; Liepins, E.; Hillers, S.
- CS Inst. Org. Sint., Riga, USSR
- SO Khimiya Geterotsiklicheskikh Soedinenii (1975), (7), 883-9 CODEN: KGSSAQ; ISSN: 0132-6244
- DT Journal
- LA Russian
- GI For diagram(s), see printed CA Issue.
- AB Nitration of Me 2-furancarboxylate by HNO3-H2SO4-Ac2O gave I-VI which were sepd. by chromatog. and identified by ir, uv, and NMR spectroscopy.

- L5 ANSWER 22 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 83:192710 CASREACT
- TI Demethylation and nitration of aryldimethilamines with cerium(IV) ammonium nitrate
- AU Galliani, Guido; Rindone, Bruno; Scolastico, Carlo
- CS Ist. Chim. Org., Univ. Milano, Milan, Italy
- SO Synthetic Communications (1975), 5(5), 319-23 CODEN: SYNCAV; ISSN: 0039-7911
- DT Journal
- LA English
- AB Treatment of Me2NPh with cerium ammonium nitrate (I) in MeOH gave 40% p-Me2NC6H4C6H4NMe2-p; in HOAc or MeCN 2,4-(O2N)2C6H3NHMe was obtained in 47 and 11% yield, resp. Treatment of p-O2NC6H4NMe2 with I in MeOH, MeCN, and HOAc, resp. gave p-O2NC6H4NHMe in 89, 60, and 23% yield, resp.; similar results were obtained for p-RC6H4NMe2 in HOAc and MeCN. A mechanism was presented for the oxidative demethylation process and the nitration reaction.
- L5 ANSWER 23 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 69:2806 CASREACT
- TI Chemistry and biochemistry of plant matter. XX. Nitration of 3',4'-dimethoxyflavanone and derivatives
- AU Reichel, Ludwig; Miller, Kurt
- CS Humboldt Univ., Berlin, Fed. Rep. Ger.
- SO Justus Liebigs Annalen der Chemie (1968), 712, 146-51 CODEN: JLACBF; ISSN: 0075-4617
- DT Journal
- LA German
- AB The course of the **nitration reaction** with fuming HNO3 and the influence of various substituents on the nitration of 3',4'-dimethoxyflavanone and its derivs. was studied. A no. of substituted 2'-hydroxynitrochalcones and their corresponding nitroflavanones were prepd. and characterized.
- L5 ANSWER 24 OF 26 CASREACT COPYRIGHT 2003 ACS
- AN 57:29296 CASREACT
- TI Synthesis of 2,2-dinitropropanol. Studies on continuous preparation
- AU Hamel, Edward E.; Dehn, John S.; Love, Joseph A.; Scigliano, Joseph J.; Swift, Arden H.
- CS Aerojet-Gen. Corp., Sacramento, CA
- SO Ind. Eng. Chem., Prod. Res. Develop. (1962), 1, 108-16
- DT Journal
- LA Unavailable
- Two routes to 2,2-dinitropropanol (I) have been evaluated as potential production processes. One route utilized the oxidative-nitration reaction of AgNO3 and NaNO2 on MeCH:CHNO2 to produce MeCH(NO2)2 (II). Treatment of II with HCHO in the presence of a basic catalyst or treatment of its salt, MeC(NO2):NO2Na, with HCHO and 1 equiv. acid produced I. Overall yields of 75% were obtained on a pilot plant scale. Ag losses (about 1%) constituted a serious drawback to large scale production. The second method (Meer, Ann. 181, 1(1876)) involved conversion of MeCHClNO2 (III) to MeC(NO2):NO2K (IV) and methylolation of IV to give I. A satisfactory prepn. of pure III was devised and a con-tinuous 4-step process was developed for I starting with nitroethane (V) with III and IV as intermediates. Although the first method gave higher yields (80% vs. 65% based on V), the second method appeared to be superior for the prepn. of large quantities of I.

- ANSWER 25 OF 26 CASREACT COPYRIGHT 2003 ACS L5
- ΑN 50:27961 CASREACT
- Alkaline nitration. I. The nitration of amines with cyanohydrin nitrates TI
- Emmons, Wm. D.; Freeman, Jeremiah P. ΑU
- Rohm & Haas Co., Huntsville, AL CS
- J. Am. Chem. Soc. (1955), 77, 4387-90 SO CODEN: JACSAT; ISSN: 0002-7863
- DT Journal
- LΑ Unavailable AΒ Me2C(CN)ONO2 (I) has been found to be a unique reagent for effecting nitration under alk. conditions. Primary and secondary amines are converted with I to the corresponding nitramines. Me2C(OH)CN (255 q.) stirred 0.5 hr. with 462 g. white fuming HNO3 (d. 1.48-1.50) in 1225 g. Ac20, the mixt. poured into 1500 cc. ice water, stirred 1 hr. intermittently, and extd. with three 300-cc. portions CH2Cl2, and the ext. washed with 200 cc. 5% aq. NaHCO3, dried, and fractionated gave 255-67 g. I, b10 65-6.degree., nD20 1.4172. iso-Bu2NH (64.5 g.) in 100 cc. MeCN treated at room temp. with 13.0 g. I in 50 cc. MeCN, the mixt. heated 4 hrs. at 80.degree., poured into 200 cc. 10% HCl, and extd. with CH2Cl2, the ext. washed with 5% aq. NaHCO3 and H2O, dried, and evapd., and the white cryst. residue recrystd. from EtOH and H2O gave iso-Bu2NNO2, shiny white platelets, m. 79-80.degree.. Morpholine (17.4 g.) treated at room temp. with 13.0 g. I, the mixt. heated 1 hr. at 80.degree., poured into dil. HCl, and extd. with CH2Cl2, the ext. dried and evapd., and the solid residue (13.0 g.) recrystd. from EtOH and H2O yielded 10.9 g. N-nitromorpholine, m. 51-3.degree.. BuNH2 (36.5 g.) in 50 cc. MeCN treated with 13.0 g. I, the mixt. refluxed 6 hrs. and worked up in the usual manner, and the residue distd. yielded 6.1 g. BuNHNO2, b0.05 68-70.degree., nD20 1.4596; the aq. exts. made alk. with Na2CO3 and extd. with Et20, and the ext. dried and distd. gave 5.6 g. .alpha.butylaminoisobutyronitrile, b8 58-9.degree., nD20 1.4286. Similarly were prepd. the following nitramines (b.p./mm., nD20, and % yield given) with I: Me2NNO2, - (m. 57-8.degree.), -, 76; Et2NNO2, 50-2.degree./0.2, 1.4525,
 60; Pr2NNO2, 90-2.degree./8, 1.4558, 42; Bu2NNO2 (II), 69-70.degree./0.1, 1.4562, 54; iso-Am2NNO2, 112-14.degree./2, 1.4604, 64; N-nitropiperidine, 62-4.degree./0.2, 1.4968, 62; N-nitropyrrolidine, - (m. 55-7.degree.), -, 60; PrNHNO2, 52-6.degree./0.1, 1.4610, 50; iso-BuNHNO2, 58-60.degree./0.1, 1.4570, 54; AmNHNO2, 60-2.degree./0.2, 1.4611, 55; iso-AmNHNO2, 62-4.degree./0.02, 1.4594, 54. Piperazine hexahydrate (III) (38.4 g.) in 100 cc. HCONMe2 heated 5 hrs. at 80.degree. with 13.0 g. I, the solvent distd. off in vacuo, the residue cooled in Dry Ice, and the resulting pale yellow solid filtered and recrystd. from EtOH yielded 7.0 g. small white platelets of mono-N-nitropiperazine, m. 127-8.degree.; it gave with PhNCS the phenylthiourea deriv., m. 204-5.degree. (from EtOH). III (38.4 g.) in 100 cc. EtOH and 50 cc. CH2Cl2 refluxed 4 hrs. with 13.0 g. I, the mixt. allowed to stand overnight, the solvent evapd., and the residue recrystd. from EtOH yielded 6.7 g. N,N'-di(.alpha.-cyanoisopropyl)piperazine, m. 178-80.degree.. III (19.4 g.) in 75 cc. HCONMe2 heated 4 hrs. at 75.degree. with 13.0 g. I, the mixt. evapd., and the solid residue recrystd. from EtOH yielded 6.8 g. N-nitro-N'-(.alpha.cyanoisopropyl)piperazine, m. 140-2.degree.. Cyclohexanone cyanohydrin (90 g.), 111 g. fuming HNO3, and 180 g. Ac2O gave in the usual manner 107.5 g. cyclohexanone cyanohydrin nitrate (IV), b0.3 62-4.degree., nD20 1.4660. Cyclopentanone (168 g.), 260 g. KCN, and 377 cc. Ac20 in 500 cc. H2O yielded 183 g. cyclopentanone cyanohydrin (V), b0.3 74-6.degree.. (183 g.), 310 g. fuming HNO3, and 837 g. Ac20 gave in the usual manner 216 g. nitrate (VI) of V, b0.25 50-1.degree., nD20 1.4592. IV (8.5 g.) and 32.3 g. Bu2NH heated 4 hrs. in 50 cc. tetrahydrofuran, the mixt. poured

into dil. HCl and extd. with Et2O, the ext. washed with 10% aq. NaHSO3, dried, and concd., and the residue distd. gave 5.0 g. II. VI (7.8 g.) and 32.3 g. Bu2NH yielded 5.5 g. II. Me2C(OH)CCl3.2H2O (21.3 g.) added during 10 min. to 102 g. Ac2O and 18.9 g. anhyd. HNO3, the mixt. stirred 0.5 hr. at room temp., quenched in 400 cc. H2O-ice mixt., and extd. with three 100-cc. portions Et2O, the ext. washed with 10% aq. Na2CO3 and H2O, dried, and evapd. in vacuo, and the residue distd. gave 20.0 g. Me2C(ONO2)CCl3, b1.0 46-50.degree., nD2O 1.481O; it did not react with piperidine. Me2C(OH)CO2Et (13.2 g.) added to 18.9 g. abs. HNO3, 51 g. Ac2O, and 30 g. AcOH, the mixt. stirred 2 hrs. at room temp., poured into ice water and extd. with CH2Cl2, and the ext. dried and distd. gave 15.9 g. Me2C(ONO2)CO2Et, b12 74-6.degree., nD2O 1.4172; it did not react with secondary amines.

=> log y		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
•	ENTRY	SESSION
FULL ESTIMATED COST	72.88	73.09
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-16.12	-16.12

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